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Quantum transport through short semiconducting nanotubes: A complex band structure analysis PAWEL POMORSKI, CHRISTOPHER MARTIN ROLAND, North Carolina State University, Raleigh, North Carolina, HONG GUO, McGill University, Montreal, Canada — Within an ab initio nonequilibrium Green's function formalism, we have examined the problem of quantum transport through short, semiconducting nanotube devices contacted with Al electrodes. Metallic behavior is predicted for very short nanotubes, which crosses over to semiconducting behavior as the tube length is increased. This behavior finds its origins in the evanescent modes that are present in these finite-sized systems, which cannot be ignored. A complex band structure analysis makes the contributions of these modes particularly transparent. Our calculation also allowed us to study the Schottky barrier formed between the nanotubes and Al contacts. We were also able to study the configuration where the whole system is in close proximity to a metal gate with some gate voltage, as is usually the case in experiment. Our computational method was able to handle metal gate boundary conditions and also implemented a numerical acceleration based on taking advantage of symmetry. References: Pawel Pomorski *et al.*, *Phys. Rev. B* **70**, 115408 (2004), Pawel Pomorski *et al.*, *Phys. Rev. B* **69**, 115418 (2004).

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